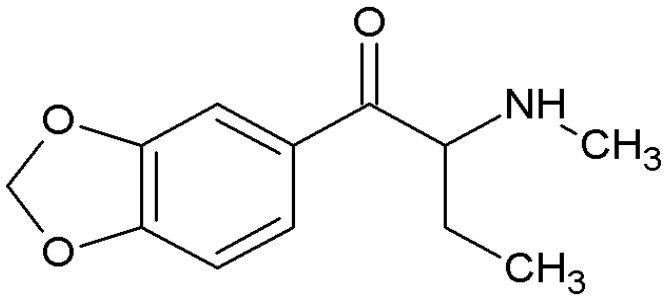
Butylone

The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.



1. GENERAL INFORMATION

IUPAC Name: 1-(1,3-Benzodioxol-5-yl)-2-(methylamino)butan-1-one

CAS #: 17762-90-2

Synonyms: *beta*-Keto-N-methylbenzodioxolylpropylamine, bk-MBDB

Source: DEA Reference Material Collection

Appearance: White powder (HCl)

UV_{max}: 234.6, 322, 282.5 nm

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	$C_{12}H_{15}NO_3$	221	Not Determined
HCl	$C_{12}H_{15}NO_3 \cdot HCl$	257	243.6

3. QUALITATIVE DATA

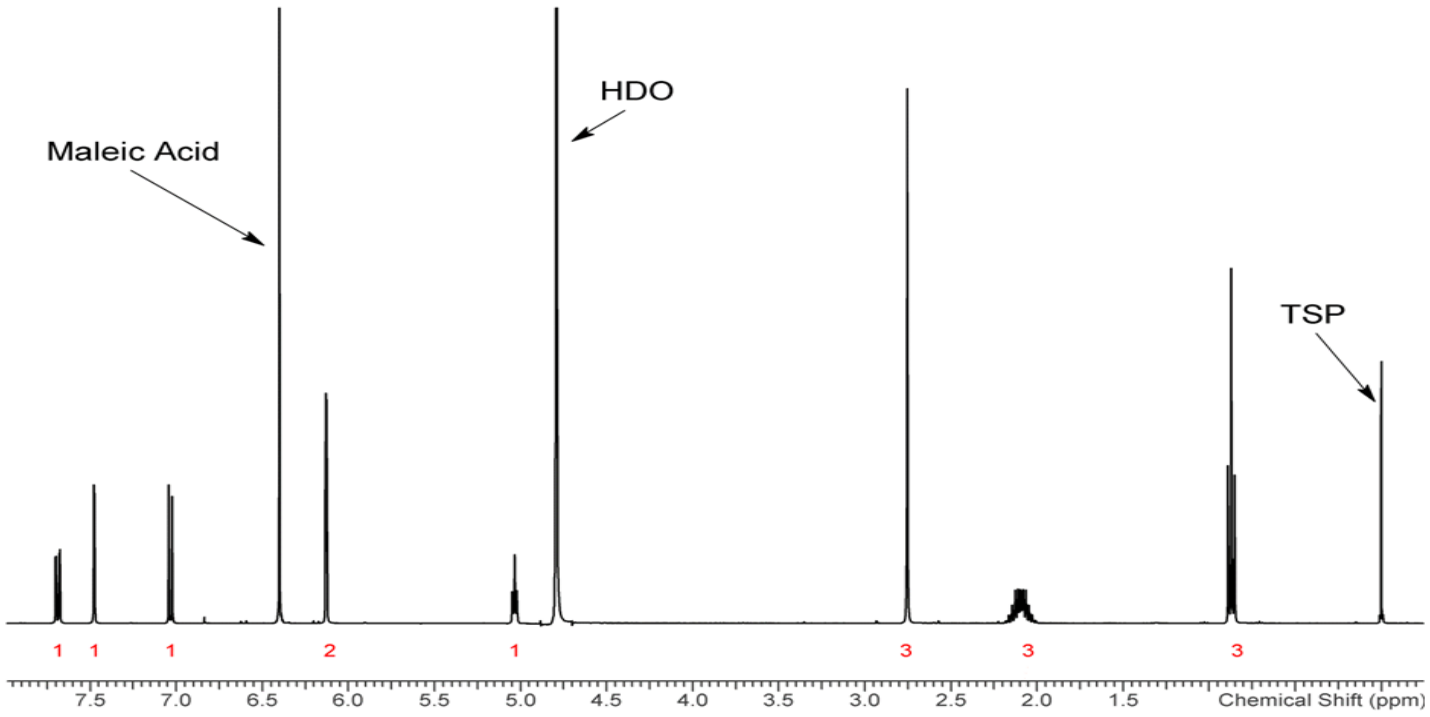
3.1 NUCLEAR MAGNETIC RESONANCE

Method NMR D_2O

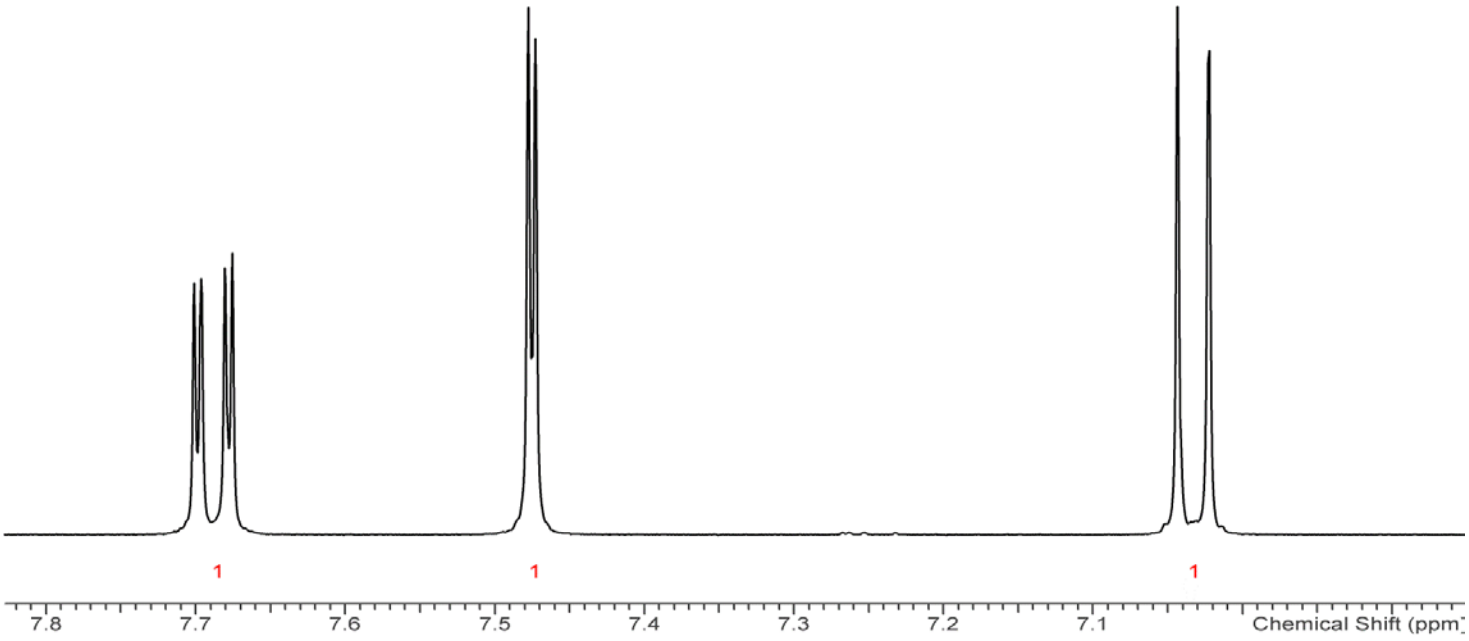
Solvent: Sample diluted to ~10 mg/mL in D_2O containing TSP for 0 ppm reference and maleic acid as quantitative ISTD

Instrument:	Varian Mercury 400 MHz NMR spectrometer with proton detection probe
Parameters:	Spectral width: at least containing -3 ppm through 13 ppm Pulse angle: 90° Delay between pulses: 45 seconds Number of scans (NT): 8 Number of steady state scans: 0 Oversampling: 4 or more Shimming: automatic gradient shimming of Z1-4 shims Phasing, Drift Correction: automatic or manual

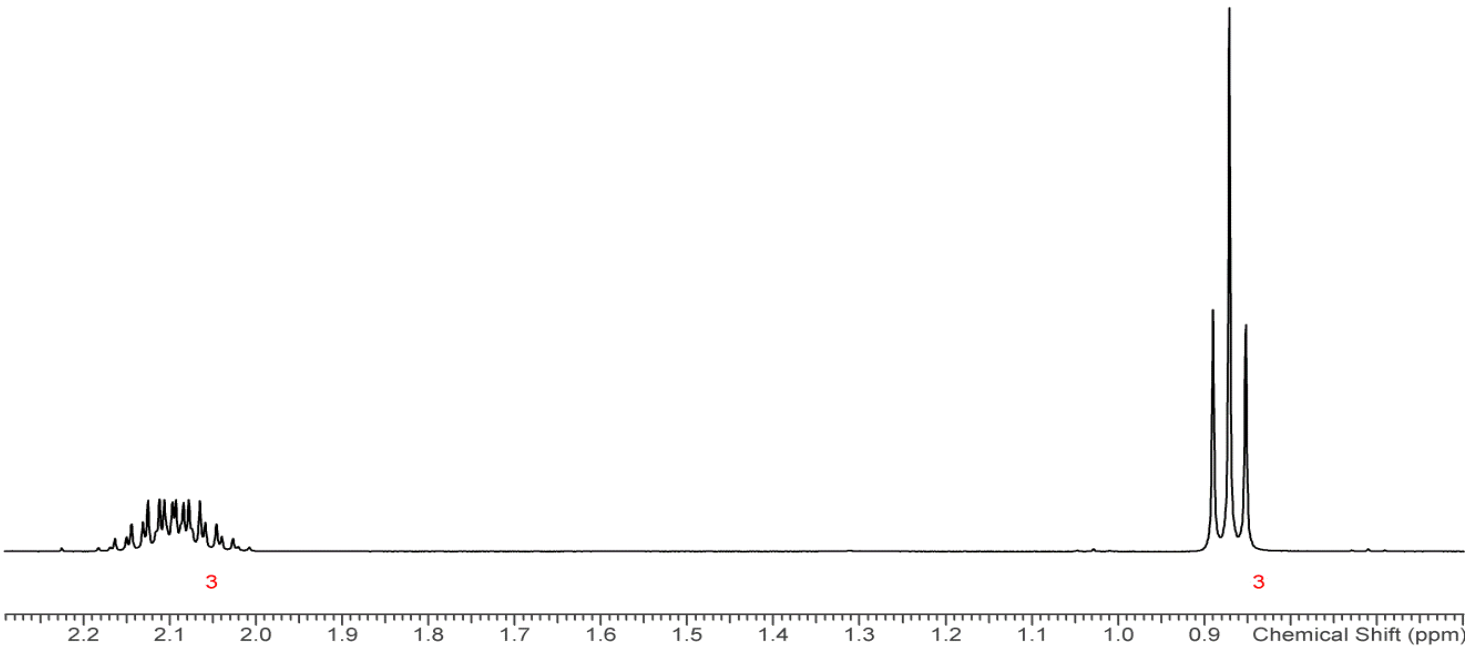
1H NMR: Butylone HCl Lot # 2011DEA003-25A D_2O, 400MHz



1H NMR: Butylone HCl Lot # 2011DEA003-25A D_2O, 400MHz



1H NMR: Butylone HCl Lot # 2011DEA003-25A D_2O, 400MHz

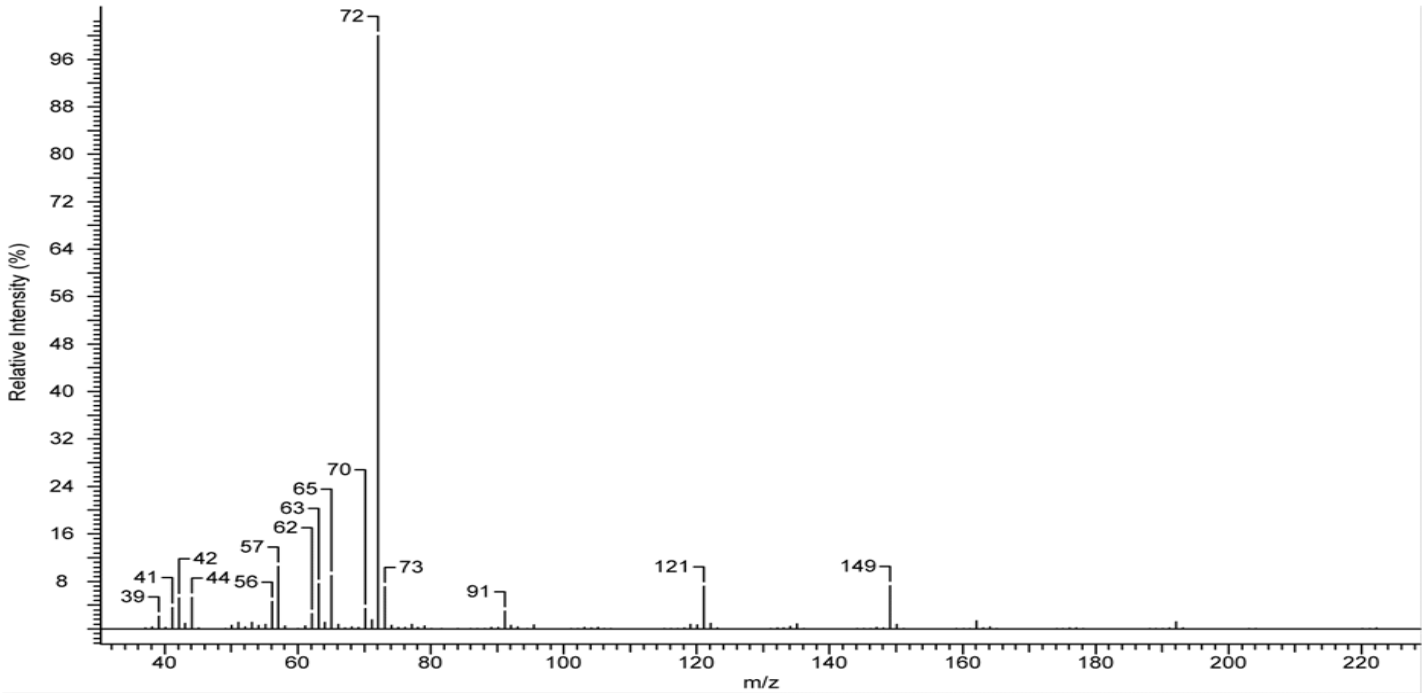


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte to ~1 mg/mL in $CHCl_3$, base extract with 1N NaOH.

Instrument:	Agilent gas chromatograph operated in split mode with MS detector
Column:	DB-1 MS; 30m x 0.25mm x 0.25µm
Carrier Gas:	Helium at 1 mL/min
Temperatures:	Injector: 280°C MSD transfer line: 280°C MS Source: 230°C MS Quad: 150°C Oven program: 1) 100°C initial temperature for 1.0 min 2) Ramp to 300°C at 12°C/min 3) Hold final temperature for 9.0 min
Injection Parameters:	Split Ratio = 25:1, 1 µL injected
MS Parameters:	Mass scan range: 34-550 amu Threshold: 100 Tune file: stune.u Acquisition mode: scan
Retention Time:	10.395 minutes

EI Mass Spectrum: Butylone HCl, Lot # 2011DEA003-25A



3.3 INFRARED SPECTROSCOPY (FTIR)

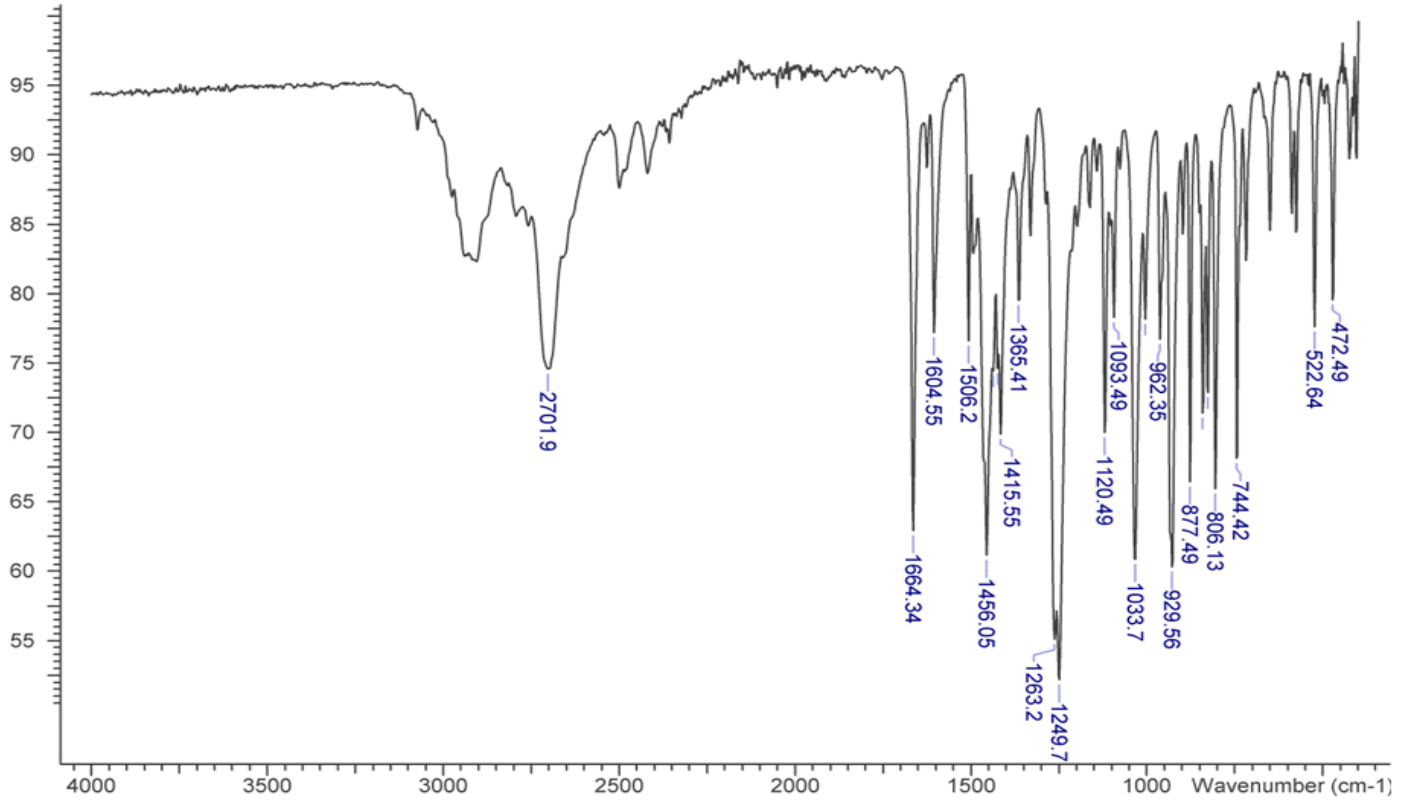
Butylone

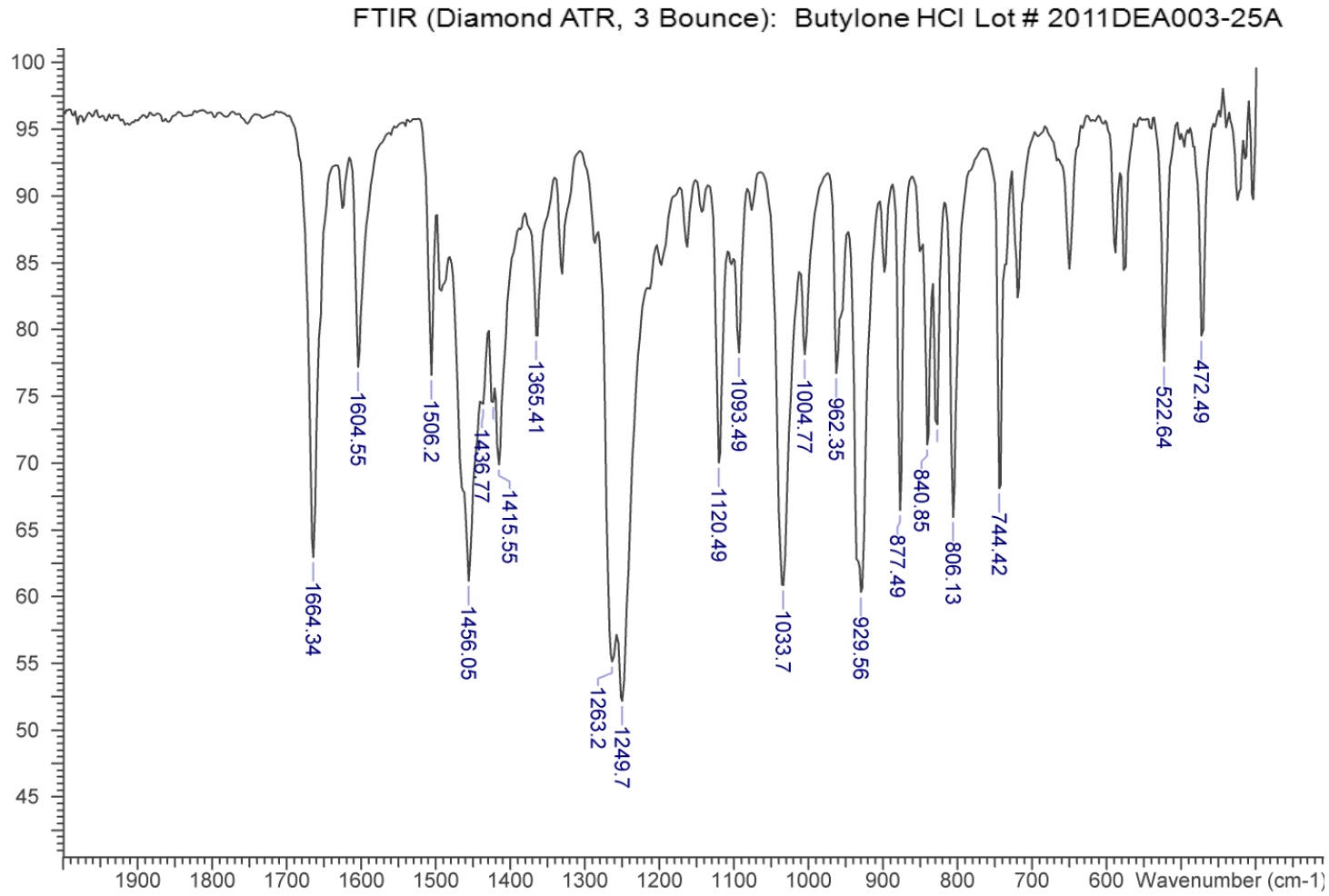
The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.

Instrument: FTIR with ATR attachment

Scan Parameters:
Number of scans: 32
Number of background scans: 32
Resolution: 4cm^{-1}
Sample gain: 8
Aperture: 150

FTIR (Diamond ATR, 3 Bounce): Butylone HCl Lot # 2011DEA003-25A





4. ADDITIONAL RESOURCES

Forendex

Wikipedia

Maheux CR, Copeland CR. Characterization of Three Methcathinone Analogs: 4-Methylmethcathinone, Methylone, and bk-MBDB. Microgram Journal 2010; 7(2):42-49.